Tridecane 629-50-5 | DTXSID6027266

Model Performance

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Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 1.55e-08 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.06e-01

Confidence level: 4.78e-01

Nearest Neighbors from the Training Set

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Tridecane

Measured: 2.55e-08 Predicted: 1.55e-08

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Tetradecane

Measured: 1.97e-08 Predicted: 1.05e-08

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Pentadecane

Measured: 3.58e-10 Predicted: 1.53e-09

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Undecane

Measured: 2.82e-08 Predicted: 1.58e-07

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Hexadecane

Measured: 3.97e-09 Predicted: 4.12e-09